Simulations of Radiation Damage Processes in Silicon Carbide

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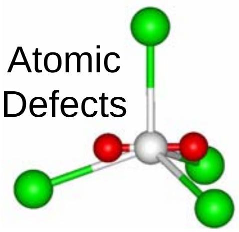
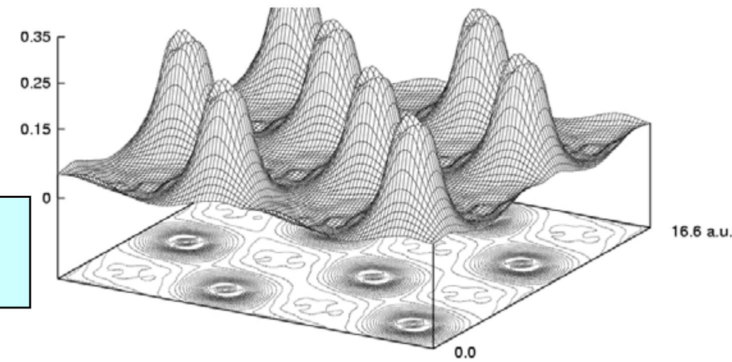
Multi-Scale Modeling of SiC

Atomic Defects

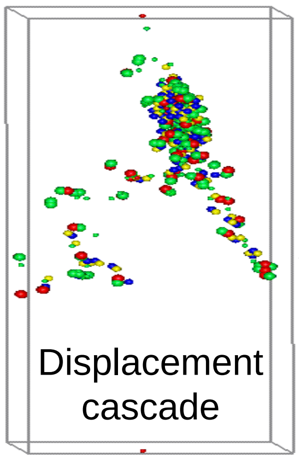


Ab initio calculations

Charge density distribution

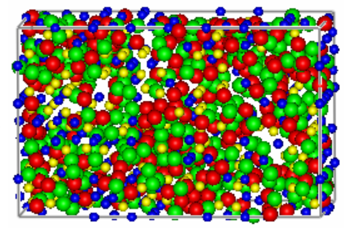


Evaluate and fit empirical potentials

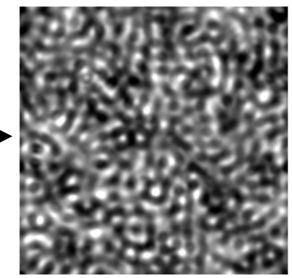


Displacement cascade

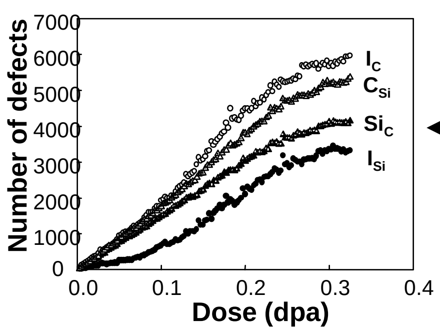
MD simulations:
Collision cascades, defect and cluster migration, binding energies, and annealing processes



Cascade Overlap



TEM Images



Defect accumulation

Kinetic Monte Carlo:
Damage accumulation and annealing

Continuum models

Experimental Observations

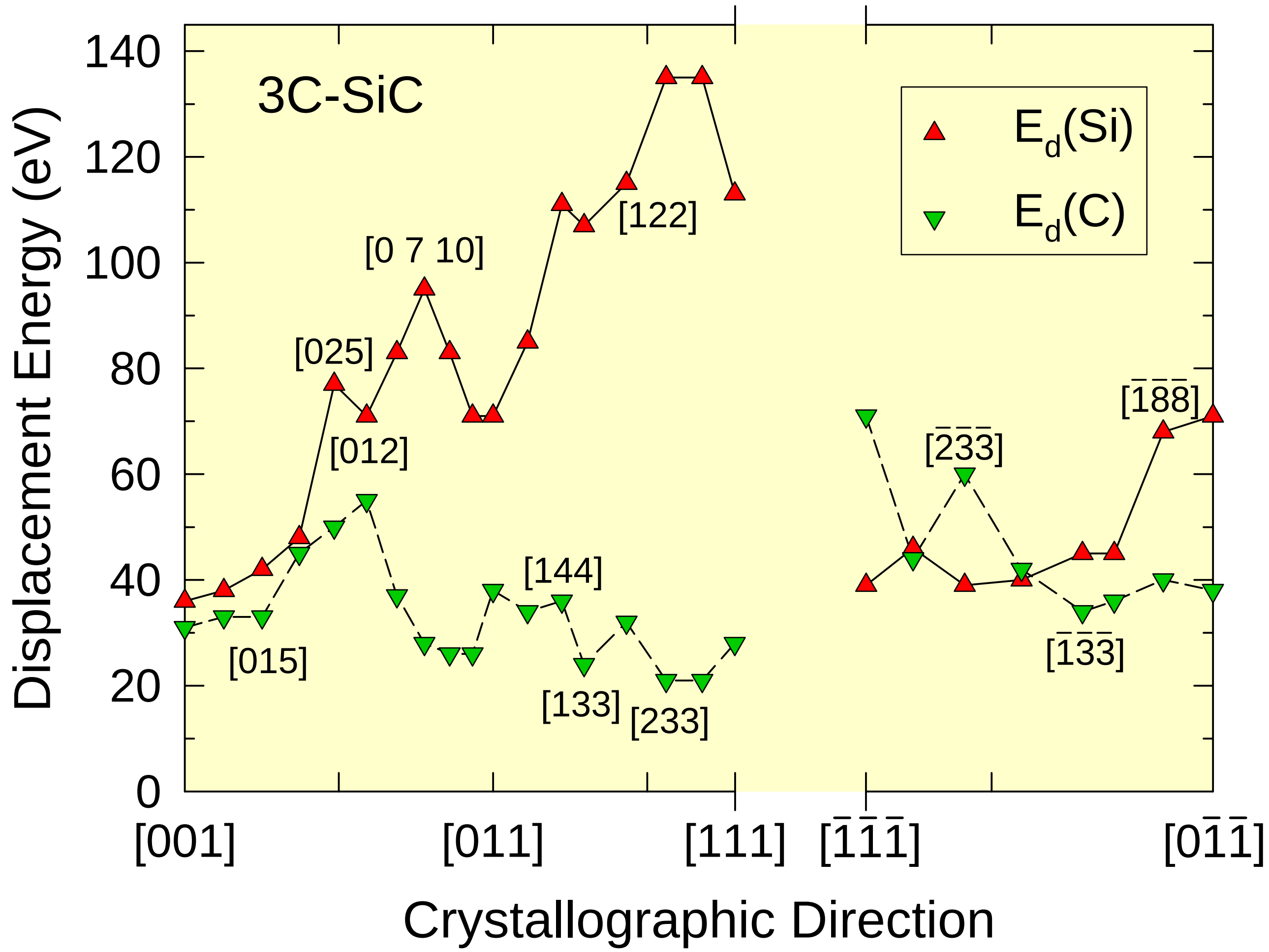
Defect Energies in 3C-SiC (MD and DFT Calculations)

Formation energies (eV)

Defect Type	MD Results	DFT Results
C^+-C<100>	3.04	3.16
C^+-Si<100>	3.43	3.59
C^+-C<110>	3.30	3.32
C^+-Si<110>	3.95	3.28
Si^+-C<100>	7.54	10.05
Si^+-Si<100>	5.53	8.32
C_{TC}	4.65	6.41
C_{TS}	4.32	5.84
Si_{TC}	3.97	6.17
Si_{TS}	6.77	8.71
C_{Si}	1.69	1.32
Si_C	4.12	7.20
V_C	2.76	5.48
V_{Si}	3.30	6.64

- Reasonable agreement between DFT & MD results for interstitials & antisites
- DFT calculations of helium-defect energies

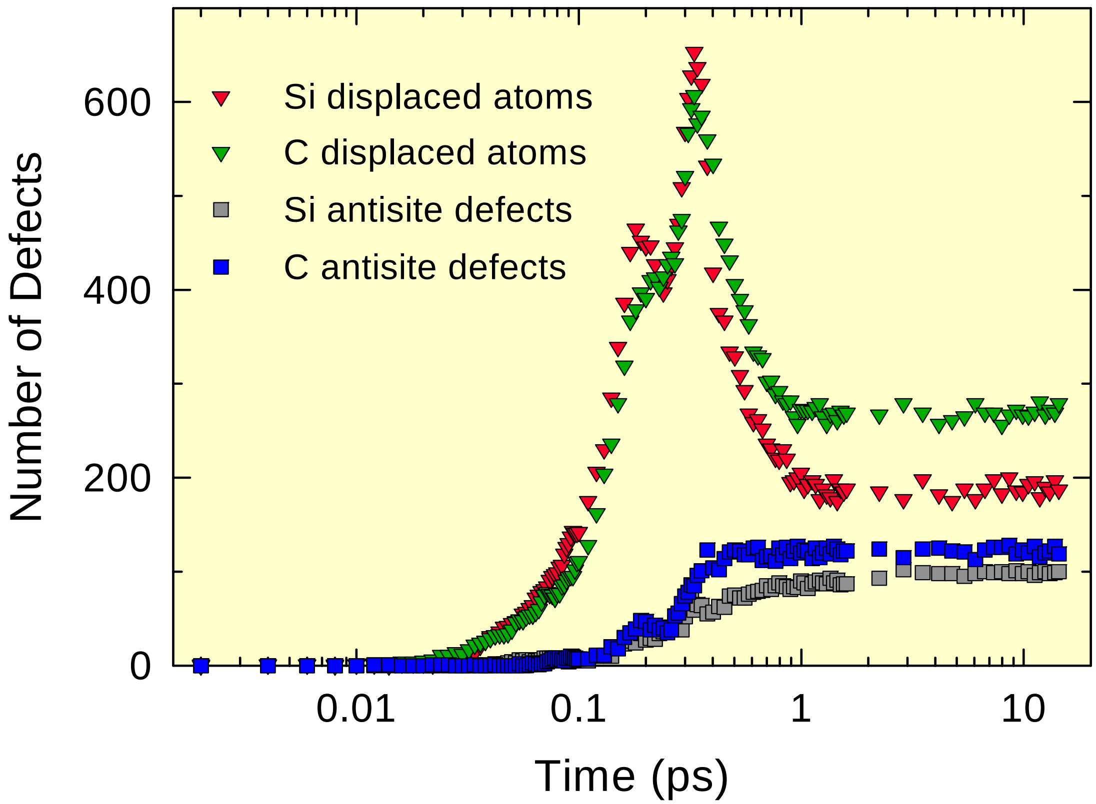
MD Results: Displacement Energy Surface for 3C-SiC

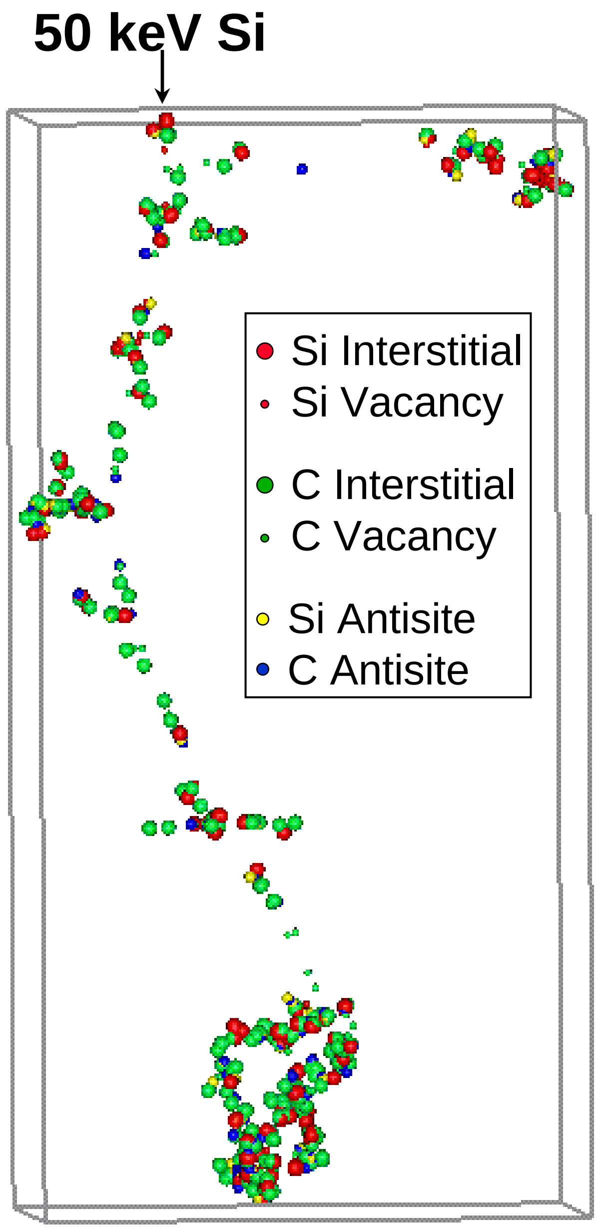


- Anisotropic; Easier to displace C; Similar results for 6H-SiC
- $E_d(Si)$ =35 eV; $E_d(C)$=20 eV; Consistent with experiments

MD Simulation of 50 keV Si Cascade in 3C-SiC

Time dependence and spatial distribution of defect production in a 50 keV Si cascade





More C defects than Si defects are produced

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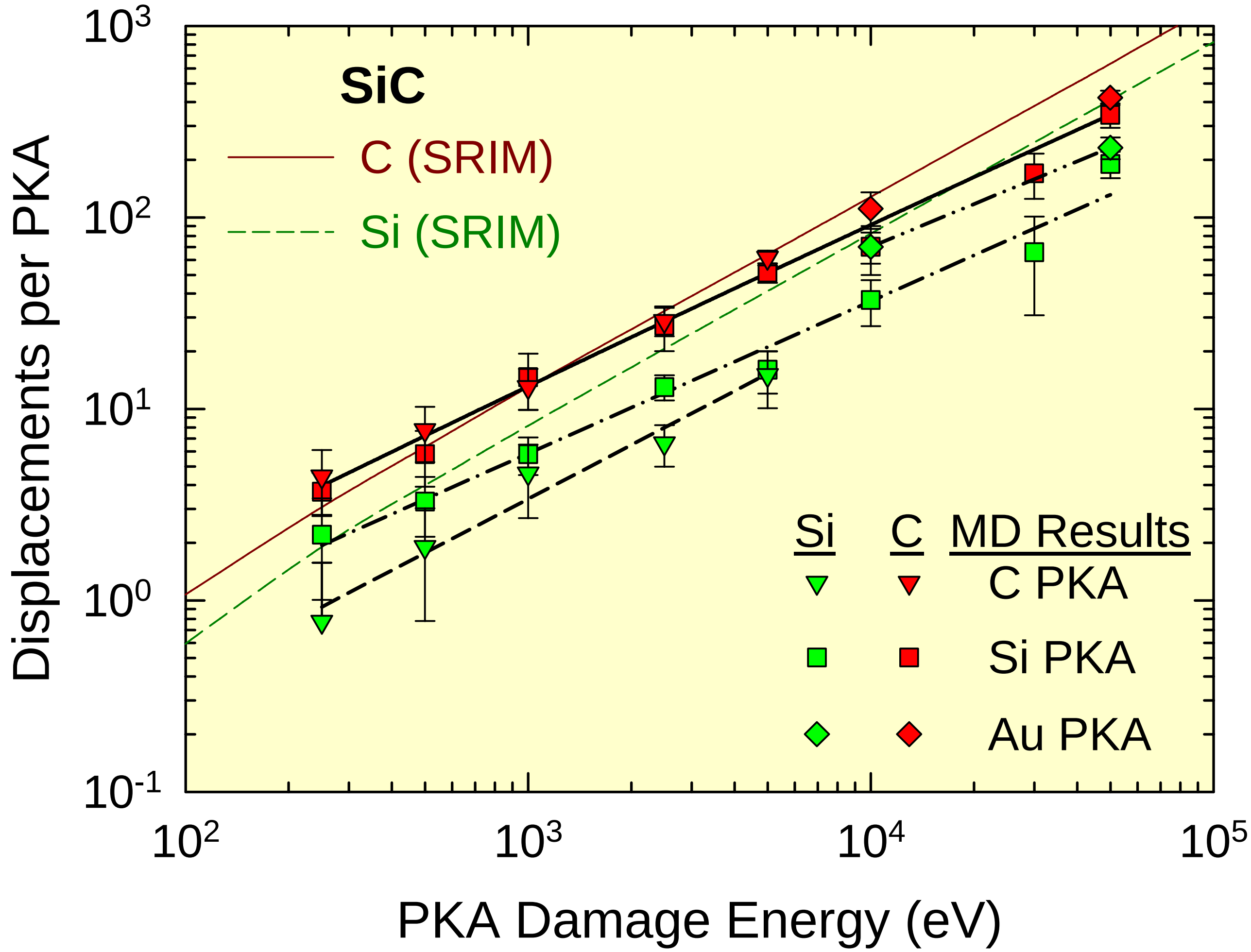
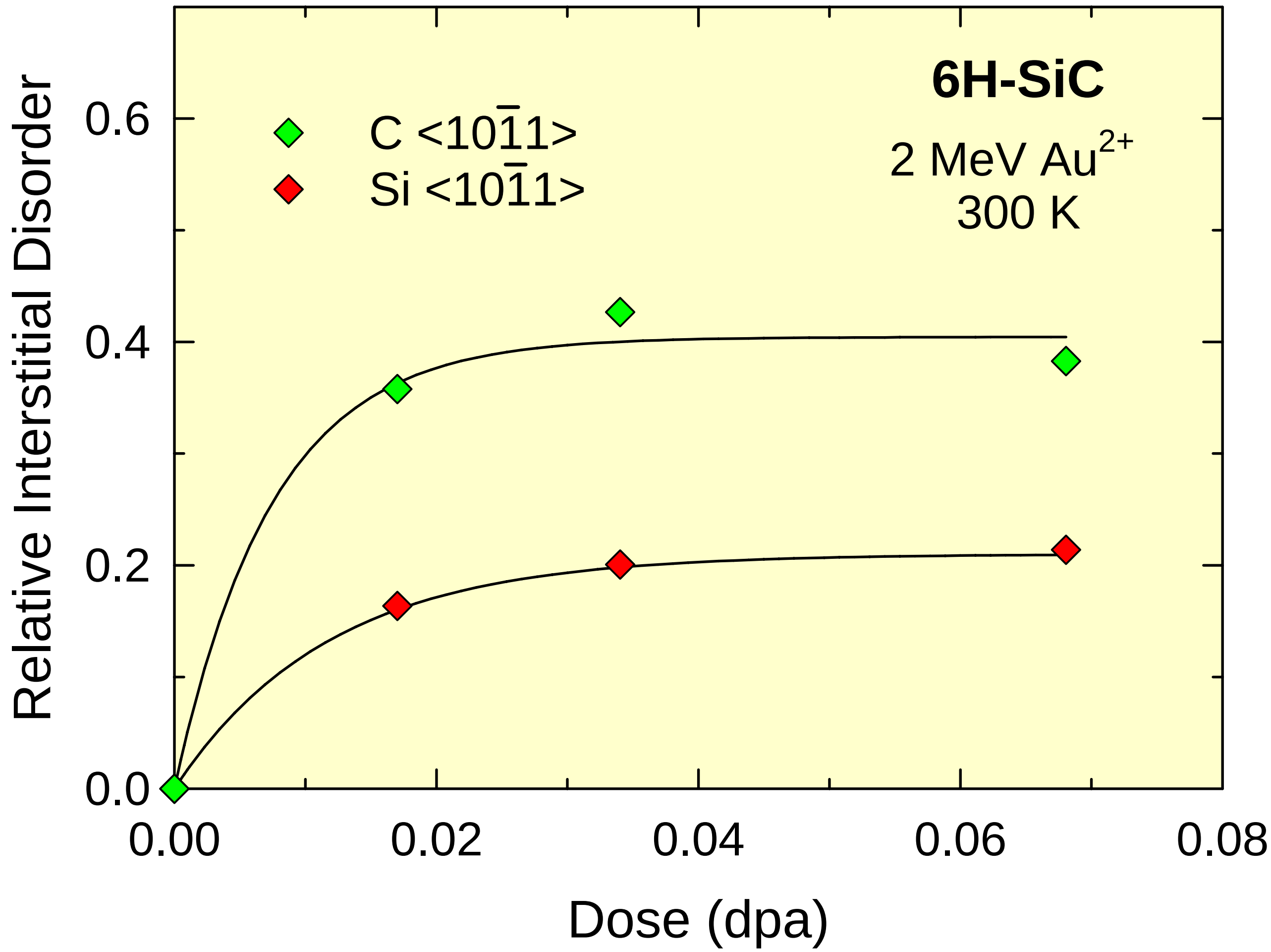
MD Results: Displacement Production vs. Damage Energy



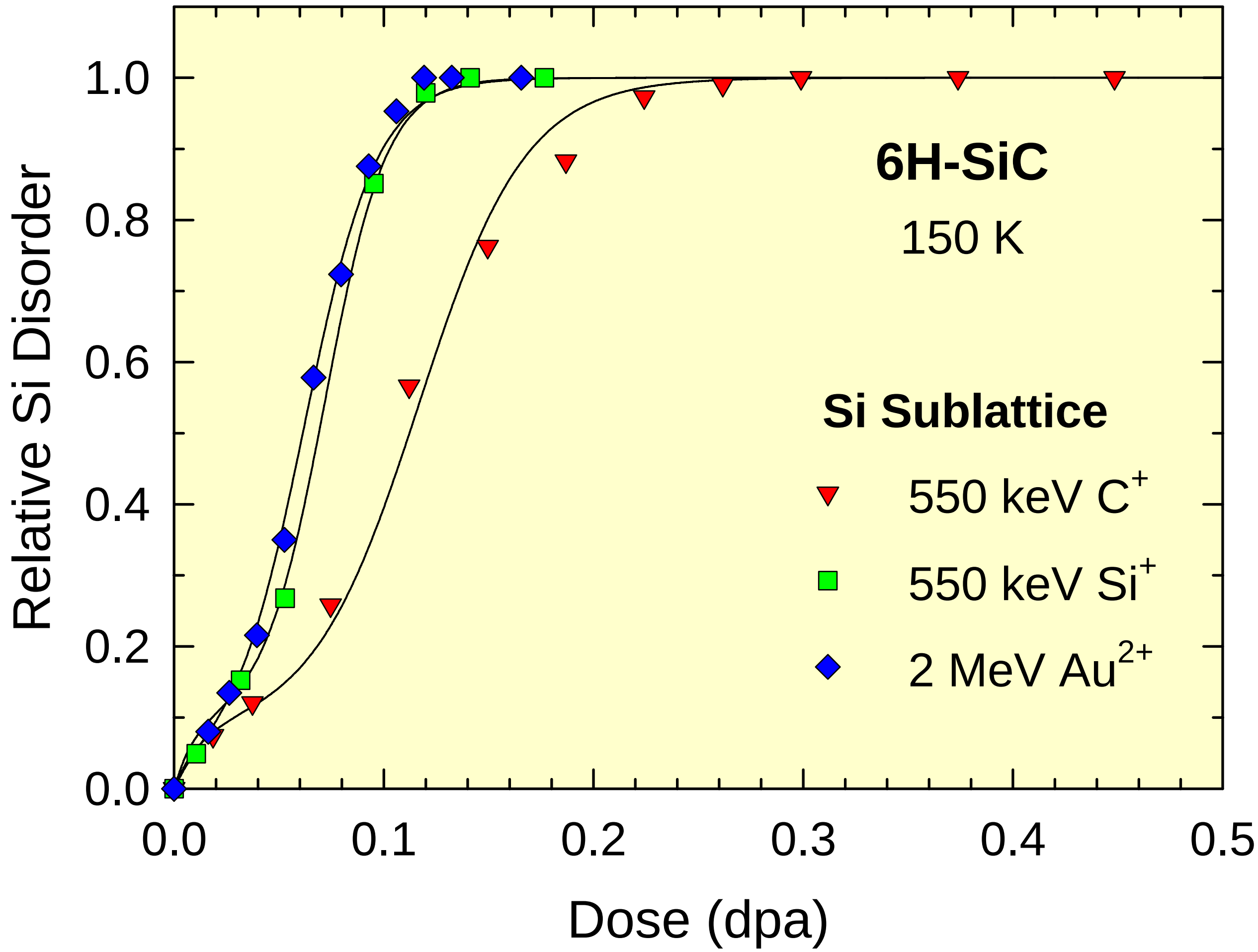
- Similar C displacement production for C, Si and Au PKAs
- Si displacement production dependent on PKA mass

Relative C & Si Disordering (at Damage Peak) in 6H-SiC



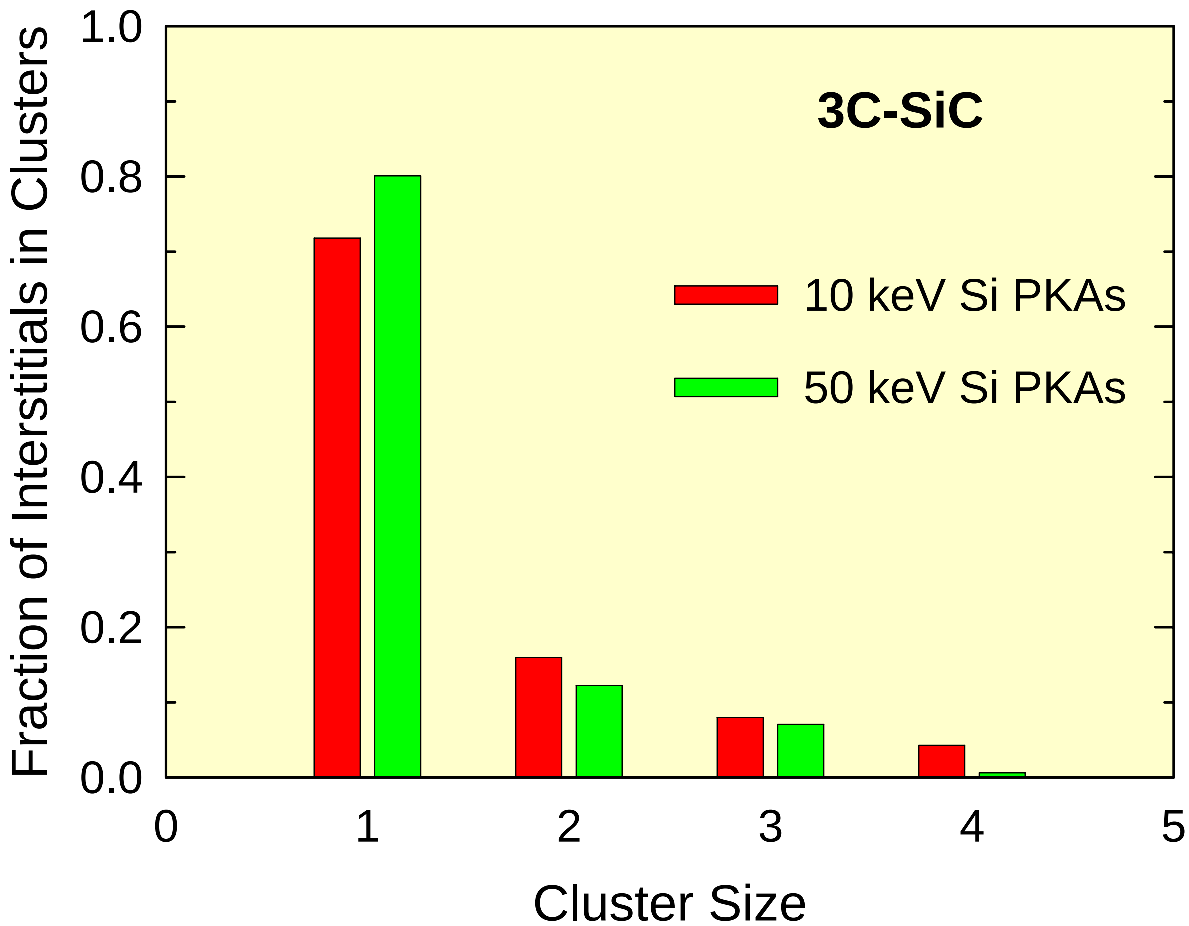
C/Si ratio at damage peak of ~ 2 is consistent with MD predictions

Si Disordering (at Damage Peak) in 6H-SiC at 150 K



For C^+ irradiation, factor of 2 lower efficiency for Si production at damage peak leads to factor of 2 lower amorphization rate

Effect of Si PKA Energy on Cluster-Size Distribution

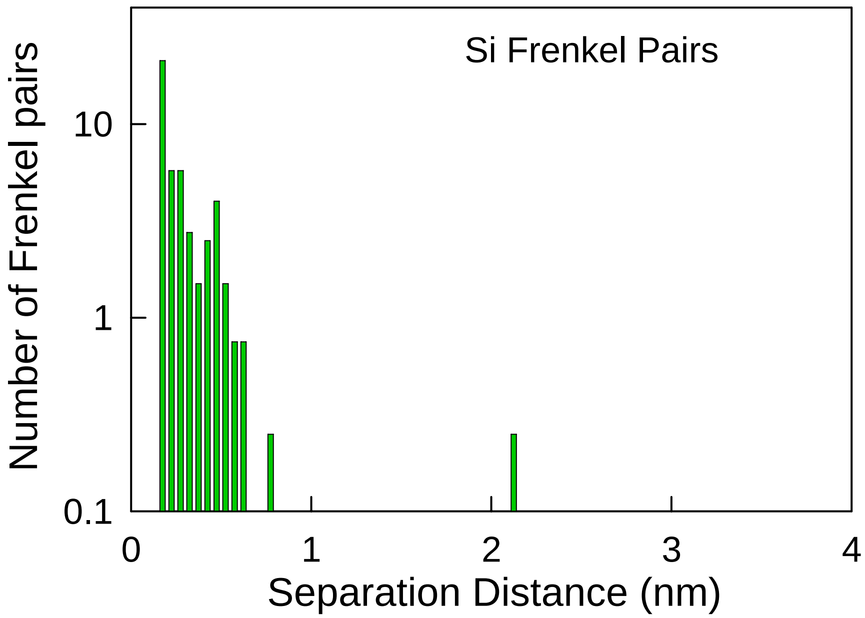


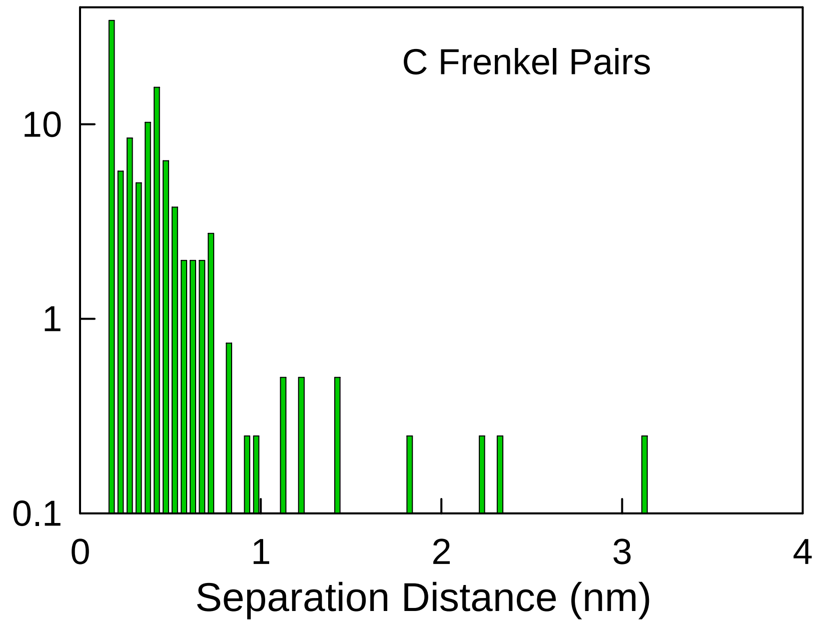
Cluster Size Distribution Not Significantly Affected by PKA Energy

All important physics is represented in 10 keV Si PKA!

Defect Displacement Distribution for Cascades in 3C-SiC

10 keV Si Cascades

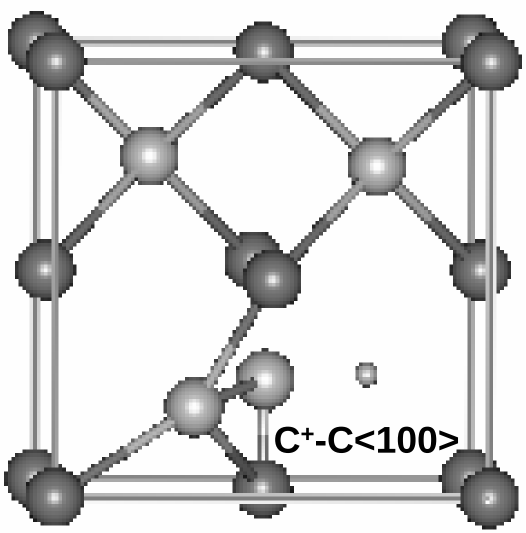


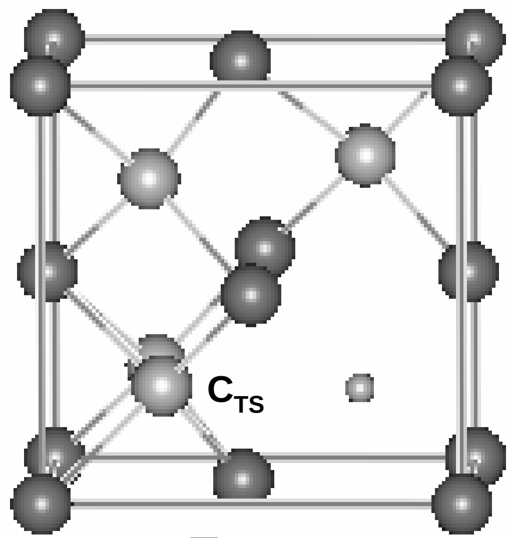


- Nearly 60% of interstitials are displaced at distances less than 0.707 a_o
- Only 40% of interstitials contribute to long-range migration processes

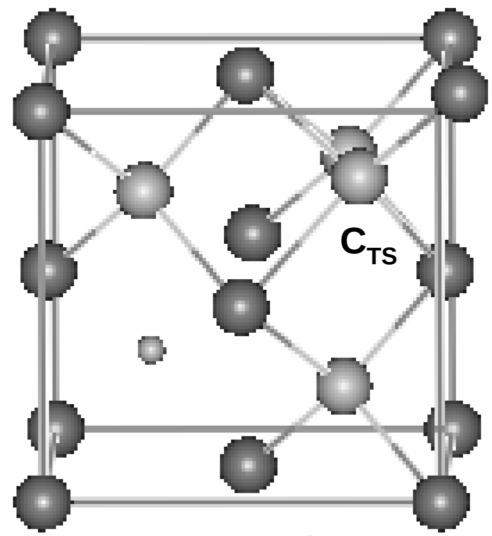
Close-Pair Recombination Kinetics in 3C-SiC

- Frenkel pairs created at low recoil energies
- Defect annealing at high temperatures (300 – 2000 K)
- Annealing times up to 100 ns
- Defect lifetime, τ, given by $\tau = \tau_o \exp(E_a/kT)$





Type a



Type b

Close-Pair Recombination Kinetics in 3C-SiC

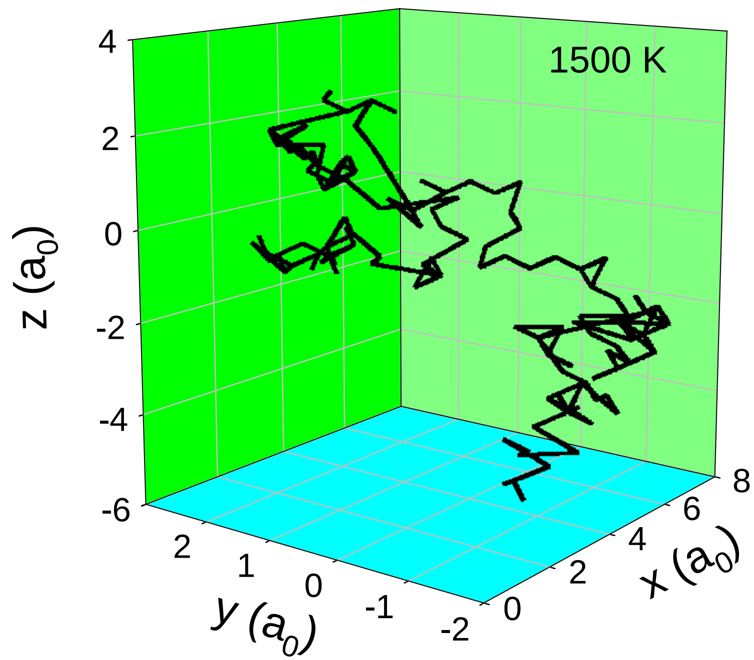
Defect Type	E_a (eV)	τ_o (ps)	d* (a_o)
C^+-C<100>	0.238	0.203	0.47
C_{TS}(a)	0.253	0.201	0.46
C_{TS}(b)	1.595	0.002	0.87
C^+-Si<100>	0.381	0.055	0.66
C^+-Si<110>	1.343	0.001	1.05
Si^+-C<100>	0.276	0.004	0.57
Si_{TC}	0.895	0.293	0.71

*d = Separation Distance of Interstitial – Vacancy pair

- E_a = 0.24 to 0.38 eV when d < 0.71 a_o (Close-Pair Recombination)
- For d > 0.71 a_o , Long-Range Diffusion Processes (larger E_a) Dominate

MD Simulation of Self-Interstitial Diffusion

Trajectory of C^+-C<100> Interstitial

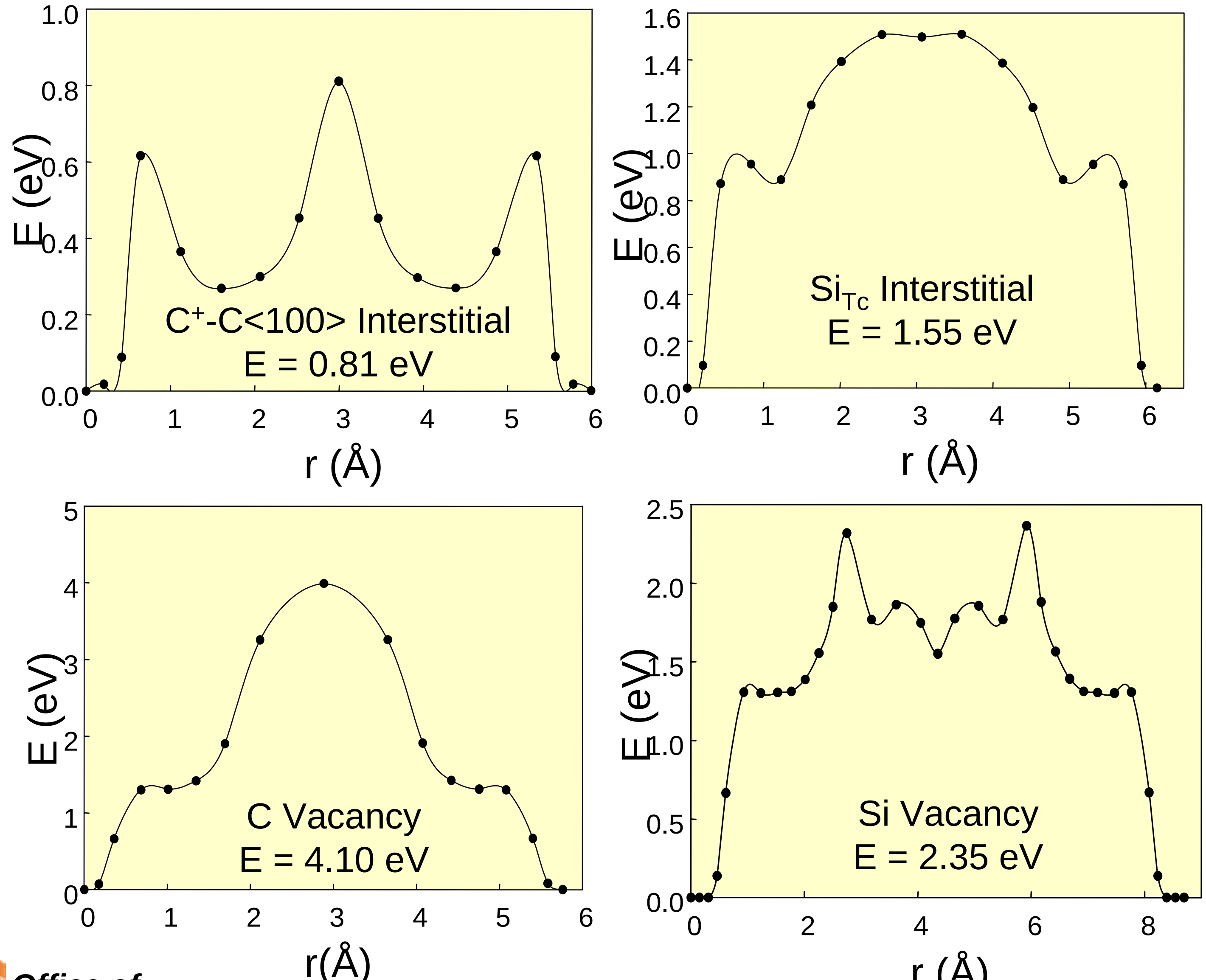


- The single interstitial diffuses three-dimensionally
- The diffusion mechanism is rather complicated

From Temperature Dependence

- Activation energy for C^+-C<100> interstitial ~ 0.74 eV
- Activation energy for Si_{TC} interstitial ~ 1.48 eV

Defect Migration Barriers: Nudged Elastic Band Method

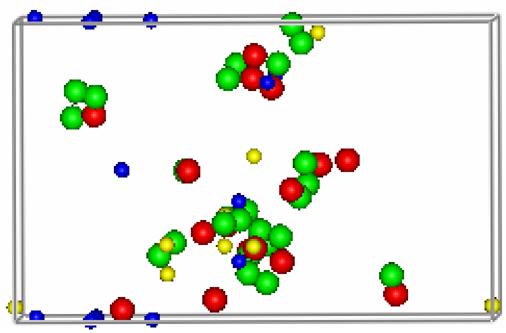


Activation Energies in SiC

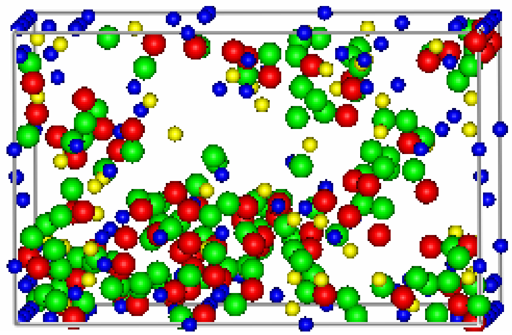
Activation Energy	Process/Mechanism
0.24 to 0.38 eV	Close-Pair Recombination
0.3 ± 0.15 eV	Stage I Recovery (6H)
0.74 – 0.81 eV	C Interstitial Migration
0.89 ± 0.20 eV	T_c (4H) (Stage II Recovery)
1.48 – 1.55 eV	Si Interstitial Migration
1.5 ± 0.3 eV; 1.6 eV	Stage III Recovery (6H)
4.10 eV	C Vacancy Migration
2.35 eV	Si Vacancy Migration

MD Simulations of Cascade Overlap Damage in SiC

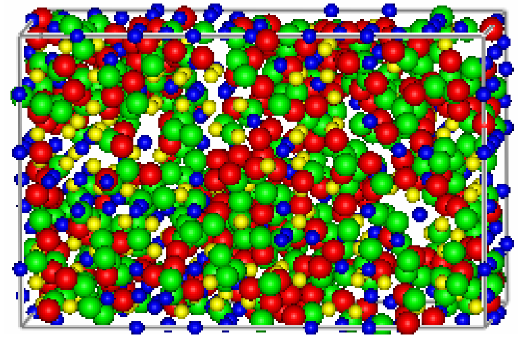
Random 10 keV Si Recoils at 200 K (Total of 140 Si Recoils)



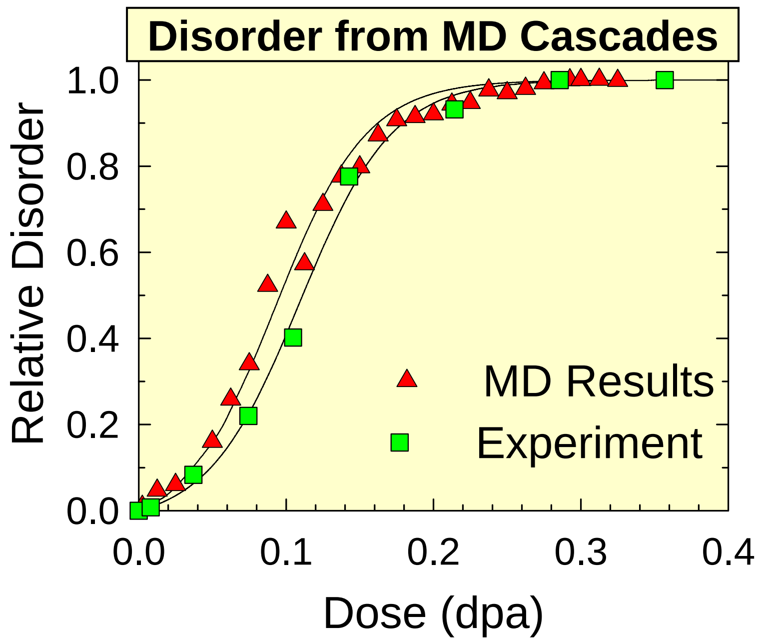
0.05 dpa

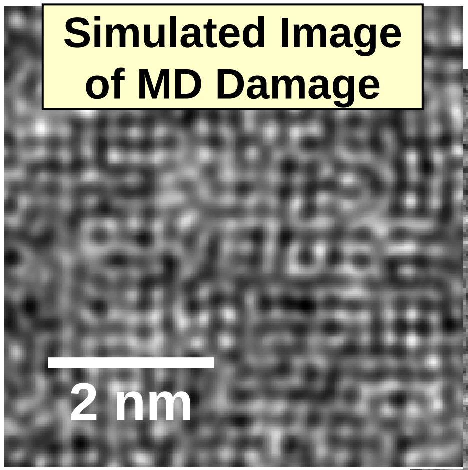


0.13 dpa

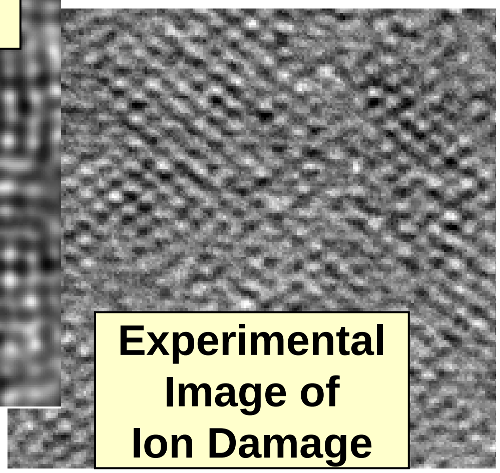


0.28 dpa





0.13 dpa



Disorder Accumulation & Simulated Images from MD are in Good Agreement with Experimental Data

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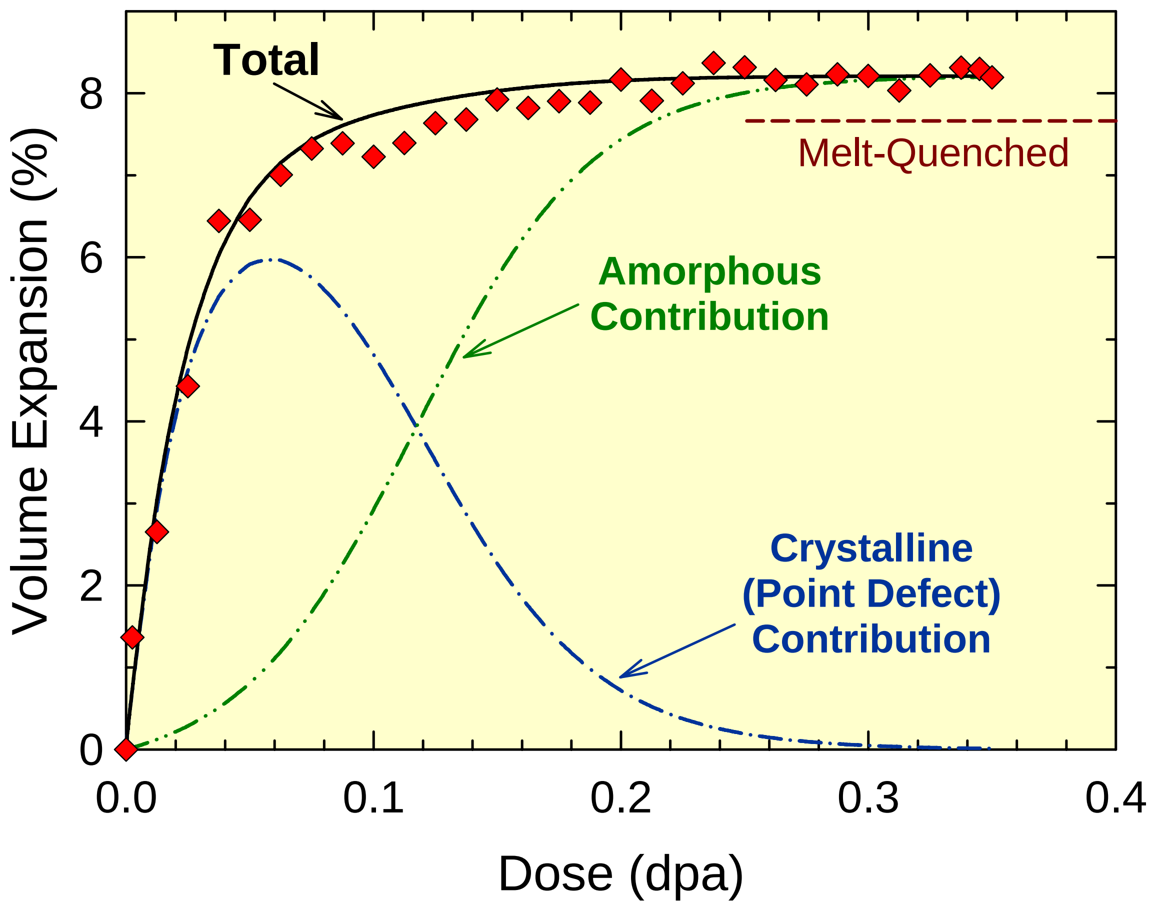
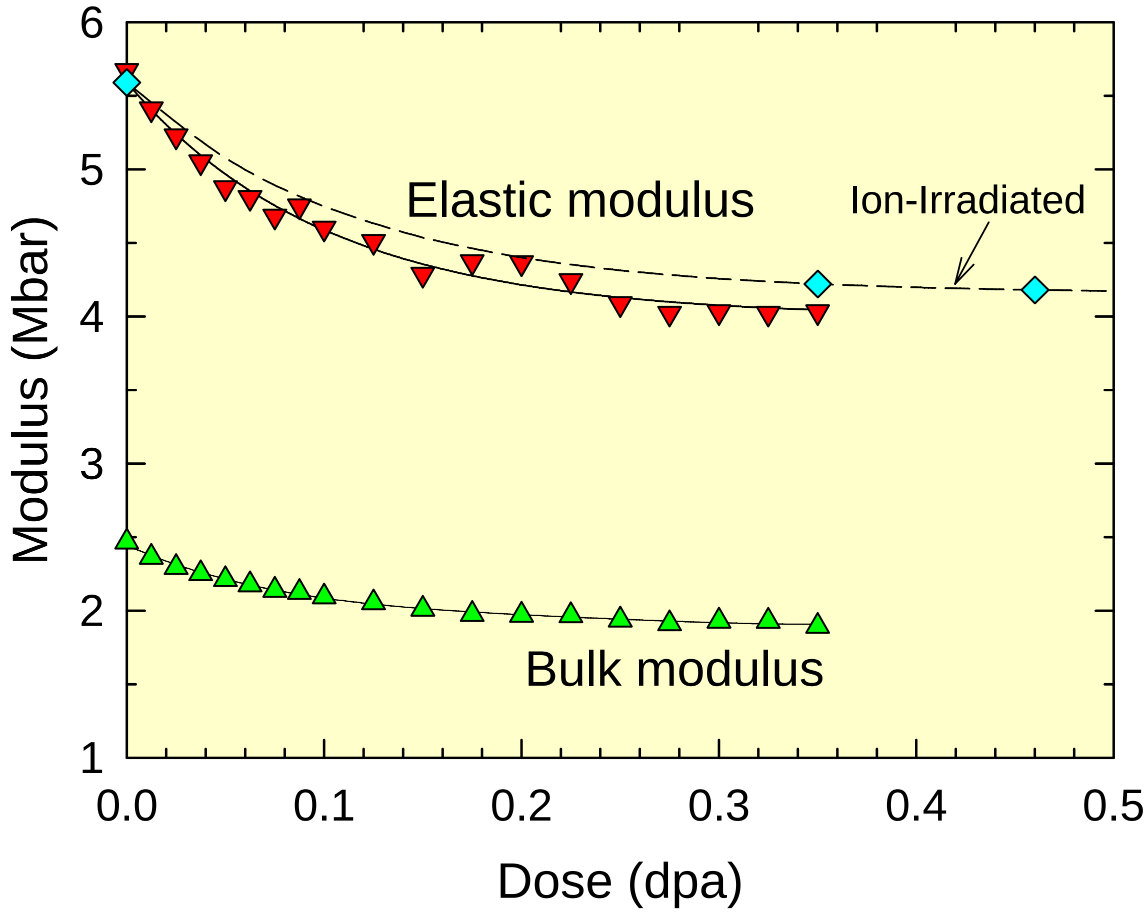
Volume Expansion from MD Cascade Overlap in SiC



- ➢ Predicted Saturation Swelling is slightly larger than the Melt-Quenched State and in reasonable agreement with experimental value of **10.8%** (Snead & Hay, 1999)
- ➢ Improvements in the Potential can yield better agreement with Experiment

Mechanical Properties Changes from MD Cascade Overlap



Changes in Elastic Modulus in Good Agreement with Experimental Results

Calculations of Changes in Thermal Conductivity from Cascade Overlap Underway

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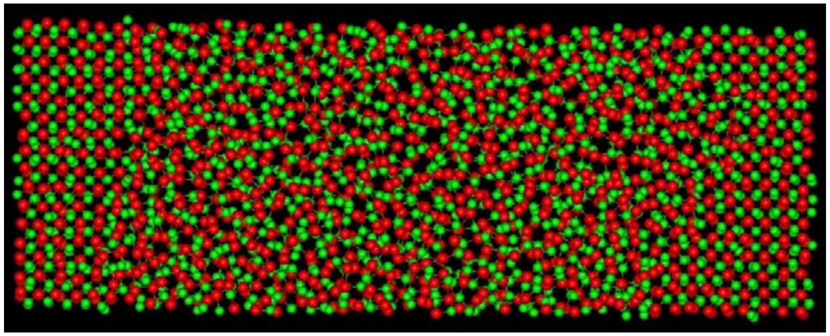
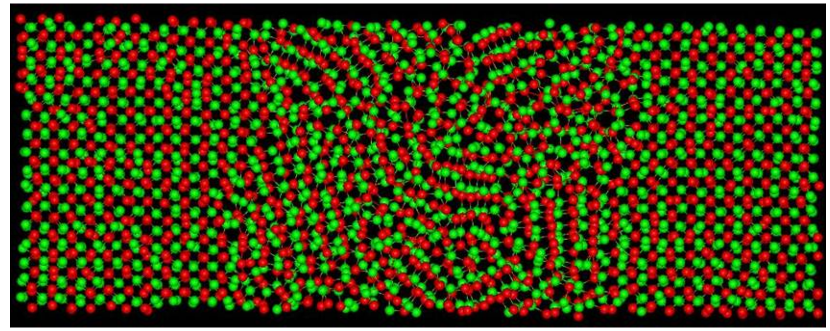
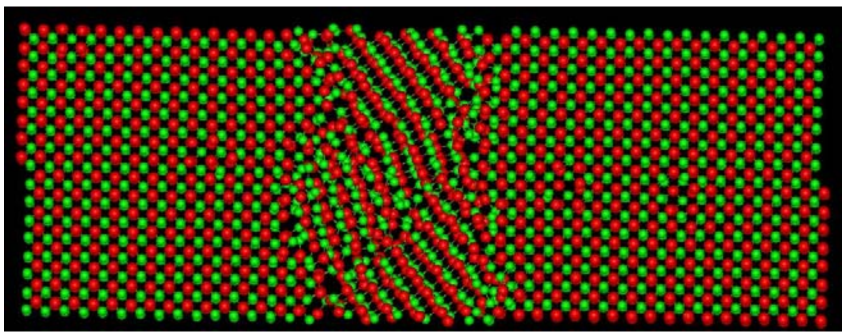
Recrystallization in 3C-SiC at 2000 K



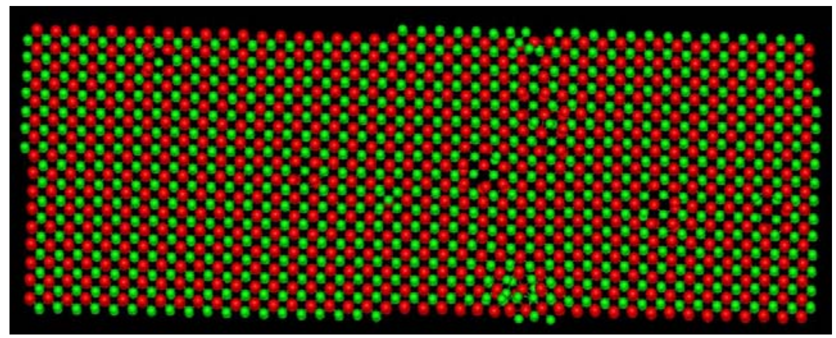
1 ns



7 ns



33 ns

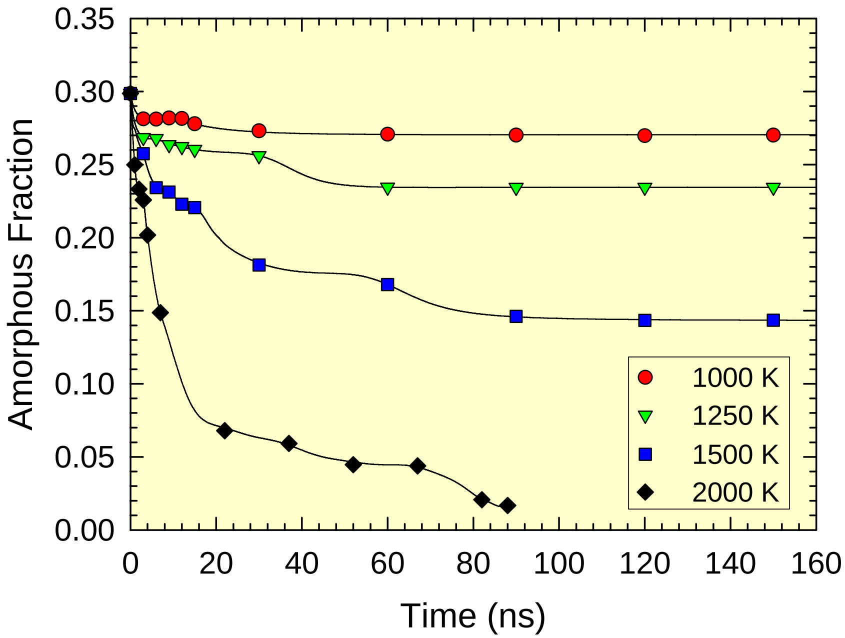


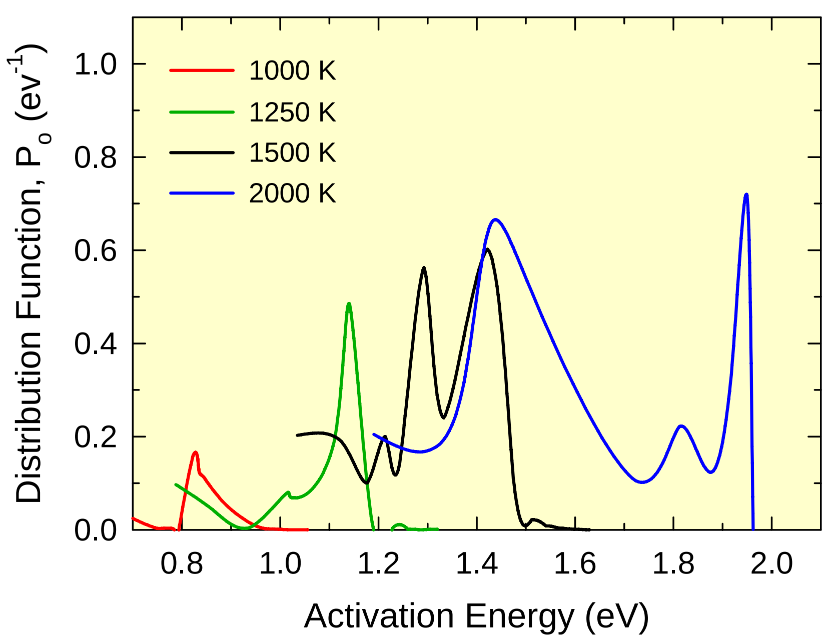
84 ns

- Initial epitaxial recrystallization of 3C-SiC
- 2H-SiC nucleates and grows as secondary phase after 33 ns
- Solid phase epitaxial regrowth of 3C phase after 84 ns

Recrystallization Dependence on Time & Temperature

Isothermal Annealing Simulations at 4 Temperatures





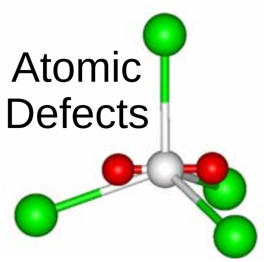
Recrystallization of the amorphous state in 3C-SiC involves multiple processes with activation energies ranging from about 0.8 to 2.0 eV

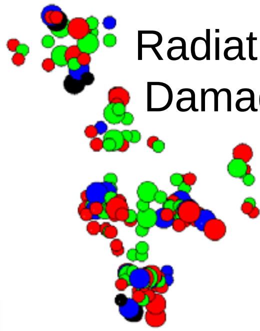
Anisotropy of Recyrstallization Processes Simulated in 4H-SiC

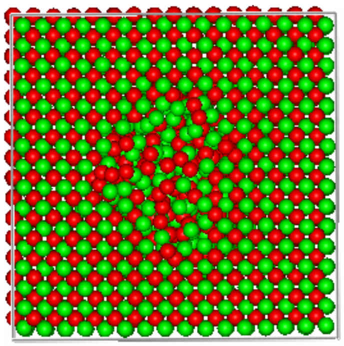
Defects and Radiation Damage Processes in SiC

Integrating Theory & Experiment to Promote Advanced Modeling

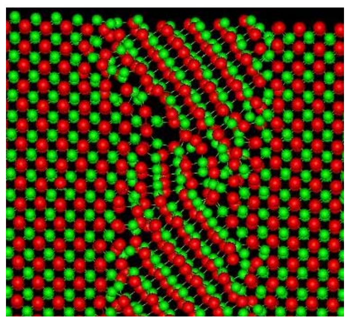
Theoretical Calculations





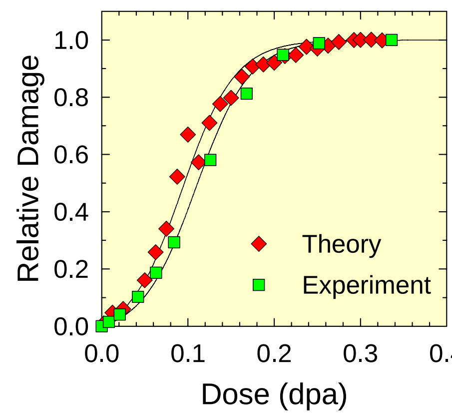


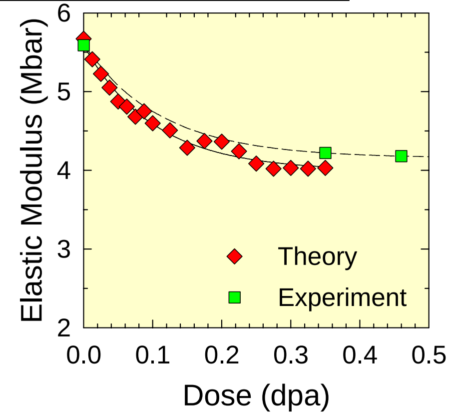
Defect Interactions



Recrystallization

Experimental Validation





Providing Understanding & Parameters necessary to Model Dynamic Evolution of Defects, Microstructure & Recrystallization in SiC as functions of Time & Temperature

- Energy-Saving Electronic Devices
- Advanced Nuclear Power
- Advanced Sensors & Detectors

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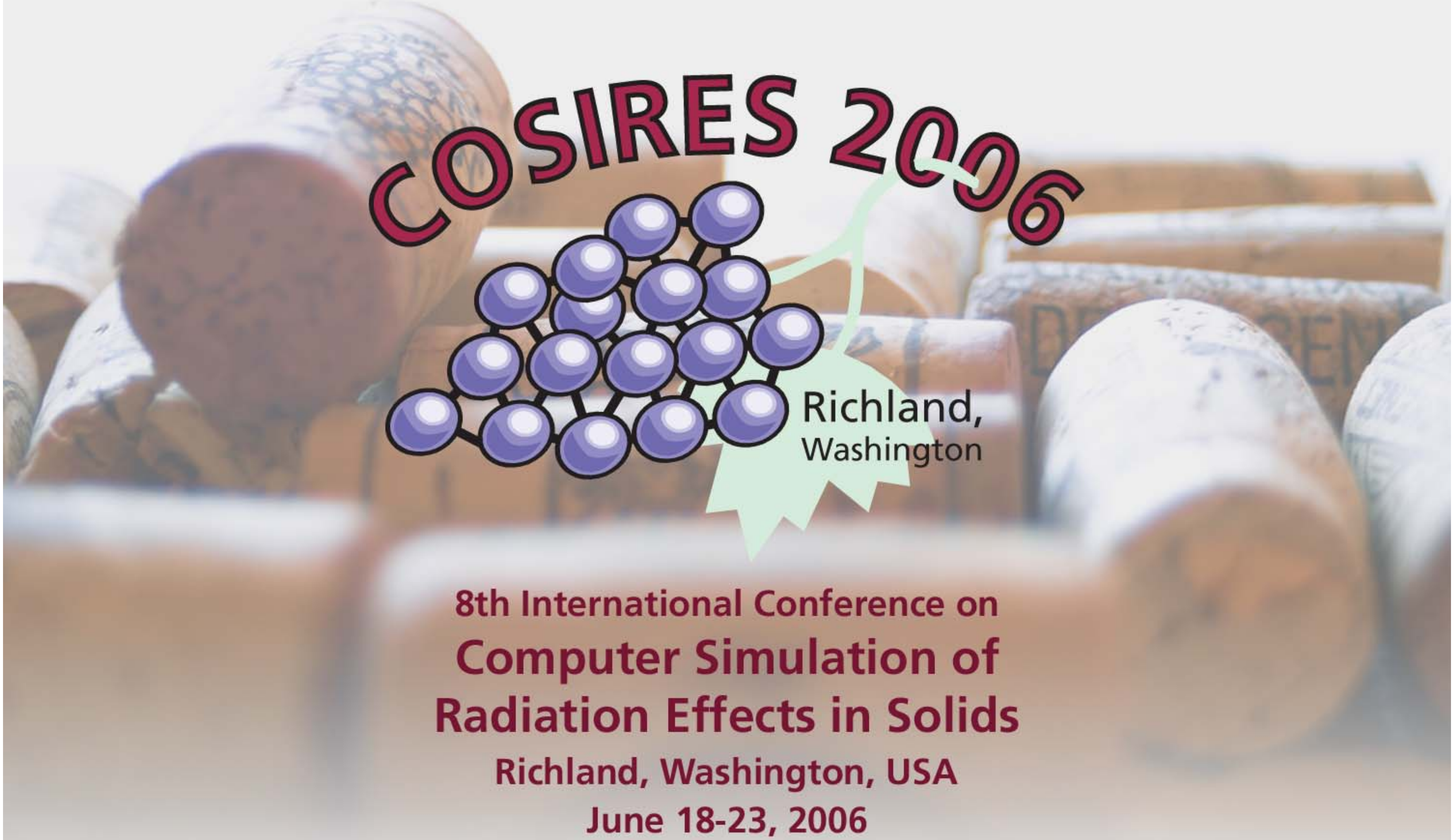

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